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TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area  
NEWS 4 Apr 09 ZDB will be removed from STN  
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB  
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available  
NEWS 9 Jun 03 New e-mail delivery for search results now available  
NEWS 10 Jun 10 MEDLINE Reload  
NEWS 11 Jun 10 PCTFULL has been reloaded  
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment  
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;  
saved answer sets no longer valid  
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY  
NEWS 15 Jul 30 NETFIRST to be removed from STN  
NEWS 16 Aug 08 CANCERLIT reload  
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 18 Aug 08 NTIS has been reloaded and enhanced  
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded  
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded  
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced  
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file  
NEWS 25 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
NEWS 26 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985  
NEWS 27 Oct 21 EVENTLINE has been reloaded  
NEWS 28 Oct 24 BEILSTEIN adds new search fields  
NEWS 29 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN  
NEWS 30 Oct 25 MEDLINE SDI run of October 8, 2002  
NEWS 31 Nov 18 DKILIT has been renamed APOLLIT  
NEWS 32 Nov 25 More calculated properties added to REGISTRY  
NEWS 33 Dec 02 TIBKAT will be removed from STN  
NEWS 34 Dec 04 CSA files on STN  
NEWS 35 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date  
NEWS 36 Dec 17 TOXCENTER enhanced with additional content  
NEWS 37 Dec 17 Adis Clinical Trials Insight now available on STN  
NEWS 38 Dec 30 ISMEC no longer available  
NEWS 39 Jan 13 Indexing added to some pre-1967 records in CA/CAPLUS  
NEWS 40 Jan 21 NUTRACEUT offering one free connect hour in February 2003  
NEWS 41 Jan 21 PHARMAML offering one free connect hour in February 2003  
NEWS 42 Jan 29 Simultaneous left and right truncation added to COMPENDEX,  
ENERGY, INSPEC  
NEWS 43 Feb 13 CANCERLIT is no longer being updated  
NEWS 44 Feb 24 METADEX enhancements  
NEWS 45 Feb 24 PCTGEN now available on STN  
NEWS 46 Feb 24 TEMA now available on STN  
NEWS 47 Feb 26 NTIS now allows simultaneous left and right truncation  
NEWS 48 Feb 26 PCTFULL now contains images

NEWS 49 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results

NEWS EXPRESS January 6 CURRENT WINDOWS VERSION IS V6.01a,  
CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:55:00 ON 13 MAR 2003

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:55:17 ON 13 MAR 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 MAR 2003 HIGHEST RN 498527-50-7  
DICTIONARY FILE UPDATES: 12 MAR 2003 HIGHEST RN 498527-50-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>  
Uploading 10027644.str

L1 STRUCTURE UPLOADED

=> s ll  
SAMPLE SEARCH INITIATED 10:56:18 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 447 TO ITERATE

100.0% PROCESSED 447 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 7672 TO 10208  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful  
FULL SEARCH INITIATED 10:56:25 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 9334 TO ITERATE

100.0% PROCESSED 9334 ITERATIONS  
SEARCH TIME: 00.00.01

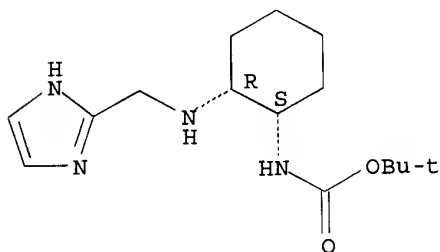
44 ANSWERS

L3 44 SEA SSS FUL L1

=> d scan

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Carbamic acid, [(1R,2S)-2-[(1H-imidazol-2-ylmethyl)amino]cyclohexyl]-,  
1,1-dimethylethyl ester, rel- (9CI)  
MF C15 H26 N4 O2

Relative stereochemistry.

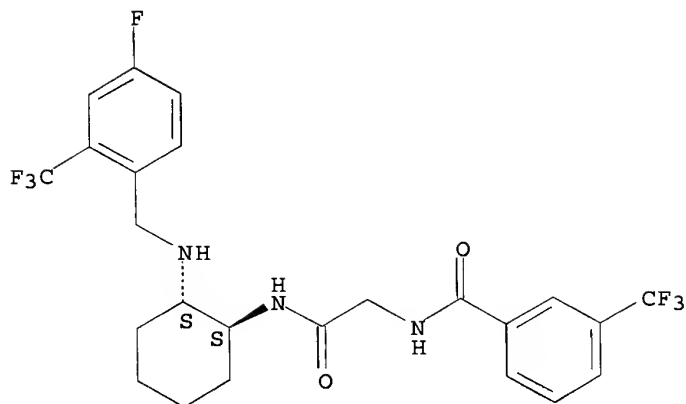


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzamide, N-[2-[[[(1S,2S)-2-[[[4-fluoro-2-(trifluoromethyl)phenyl]methyl]a  
mino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI)  
MF C24 H24 F7 N3 O2

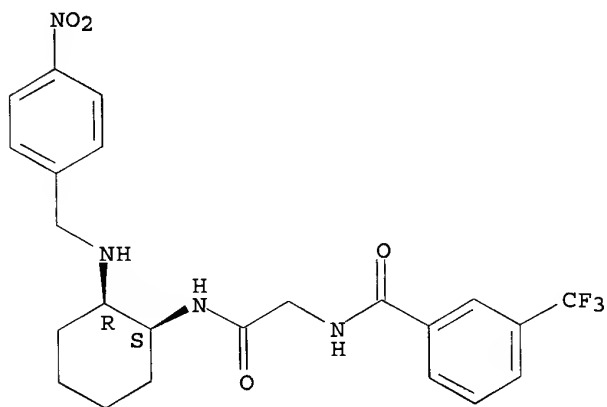
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, N-[2-[[[(1R,2S)-2-[[[4-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)phenyl]-, rel- (9CI)  
 MF C23 H25 F3 N4 O4

Relative stereochemistry.

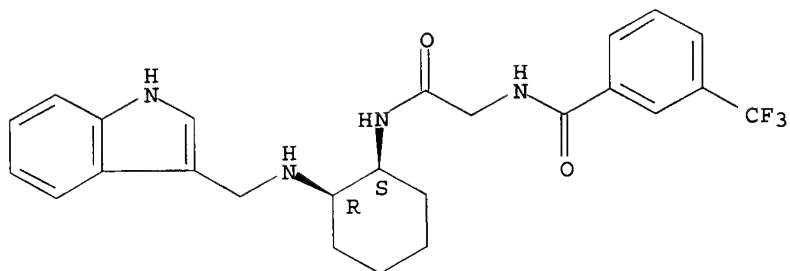


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, N-[2-[[[(1R,2S)-2-[[[4-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)phenyl]-, rel- (9CI)  
 MF C25 H27 F3 N4 O2

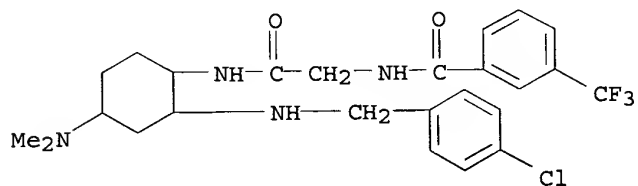
Relative stereochemistry.



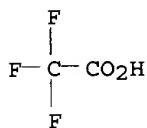
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzamide, N-[2-[[2-[[[4-chlorophenyl)methyl]amino]-4-(dimethylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI)  
 MF C25 H30 Cl F3 N4 O2 . x C2 H F3 O2

CM 1



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.95

149.16

FILE 'CAPLUS' ENTERED AT 10:56:48 ON 13 MAR 2003

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FILE COVERS 1907 - 13 Mar 2003 VOL 138 ISS 11  
FILE LAST UPDATED: 12 Mar 2003 (20030312/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> hist dis

HIST IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> dis his

(FILE 'HOME' ENTERED AT 10:55:00 ON 13 MAR 2003)

FILE 'REGISTRY' ENTERED AT 10:55:17 ON 13 MAR 2003

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 44 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:56:48 ON 13 MAR 2003

=> s l3

L4 8 L3

=> d l4 ibib hitstr abs 1-8

L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:594806 CAPLUS

DOCUMENT NUMBER: 137:154762

TITLE: Preparation of N-[2-(cycloalkylamino)-2-oxoethyl]benzamides and related compounds as modulators of chemokine receptor activity

INVENTOR(S): Cherney, Robert

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 286 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

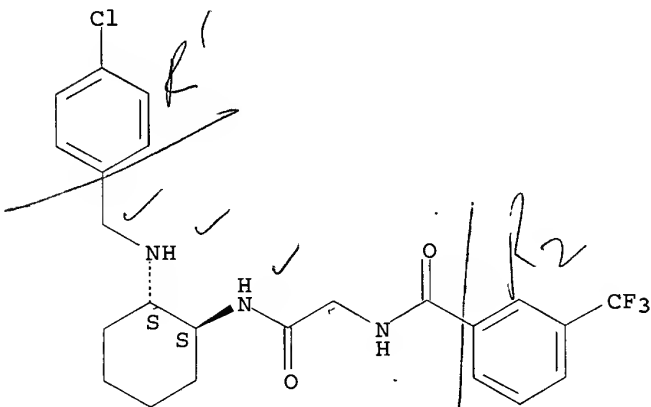
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002060859	A2	20020808	WO 2001-US50252	20011220
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, <u>GO, GW, ML</u> , MR, NE, SN, TD, TG			
US 2003004151	A1	20030102	US 2001-27644	20011220
PRIORITY APPLN. INFO.:			US 2000-256904P	P 20001220
OTHER SOURCE(S):		MARPAT 137:154762		

IT **445478-71-7P**, N-[2-[[[(1S,2S)-2-[[[(4-Chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (chemokine receptor modulator; prepn. of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)  
 RN **445478-71-7** CAPLUS  
 CN Benzamide, N-[2-[[[(1S,2S)-2-[[[(4-chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **445478-74-0P**, N-[2-[[[(1S,2S)-2-[[[(2,4-Dimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-75-1P**, N-[2-[[[(1S,2S)-2-[[[(2,4,6-Trimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-76-2P**, N-[2-[[[(1S,2S)-2-[[[(4-Benzyloxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-77-3P**, N-[2-[[[(1S,2S)-2-[[[(2,4-Difluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-78-4P**, N-[2-[[[(1S,2S)-2-[[[(2-Chloro-4-fluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-79-5P**, N-[2-[[[(1S,2S)-2-[[[(2-Trifluoromethyl-4-fluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-80-8P**, N-[2-[[[(1S,2S)-2-[[[(2,4-Dichlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-81-9P**, N-[2-[[[(1S,2S)-2-[[[(2-Fluoro-6-trifluoromethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-82-0P**, N-[2-[[[(1S,2S)-2-[[[(2-Chloro-5-trifluoromethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-83-1P**, N-[2-[[[(1S,2S)-2-[[[(1-Naphthyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-87-5P**, N-[2-[[[cis-2-[[[(2,4-Dimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-88-6P**, N-[2-[[[cis-2-[[[(4-Chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-89-7P**, N-[2-[[[cis-2-[[[(4-Nitrophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-90-0P**, N-[2-[[[cis-2-[[[(4-Isopropylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-91-1P**, N-[2-[[[cis-2-[[[(4-Trifluoromethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-92-2P**, N-[2-[[[cis-2-[[[(4-Trifluoromethoxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-

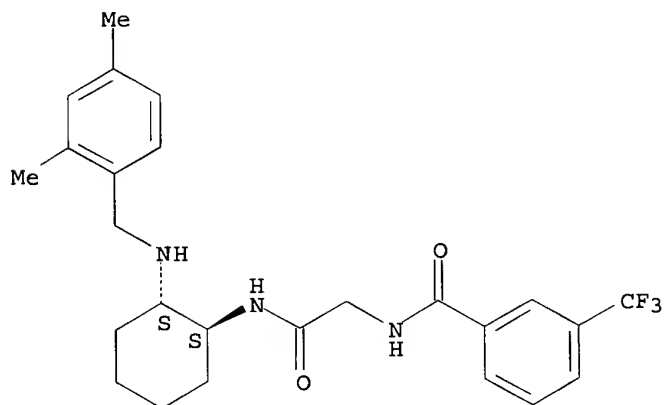
(trifluoromethyl)benzamide **445478-93-3P**, N-[2-[[cis-2-[[4-Phenoxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-94-4P**, N-[2-[[cis-2-[[1-Naphthyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-95-5P**, N-[2-[[cis-2-[[2-Naphthyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-96-6P**, N-[2-[[cis-2-[[3-Indolyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445480-70-6P**, 2-Isopropylamino-N-[[[cis-2-(4-methylthiobenzylamino) cyclohexyl] carbamoyl]methyl]-5-(trifluoromethyl)benzamide **445480-72-8P 445480-74-0P 445481-10-7P 445481-16-3P 445481-18-5P 445481-20-9P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(chemokine receptor modulator; prepn. of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

RN 445478-74-0 CAPLUS  
CN Benzamide, N-[2-[[[(1S,2S)-2-[[[(2,4-dimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

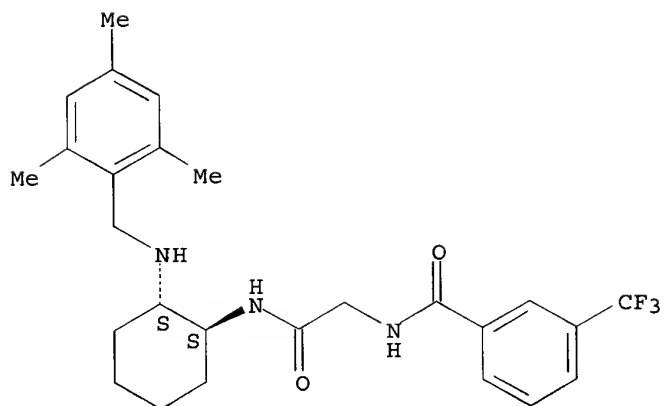
Absolute stereochemistry.



RN 445478-75-1 CAPLUS  
CN Benzamide, N-[2-oxo-2-[[[(1S,2S)-2-[[[(2,4,6-trimethylphenyl)methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

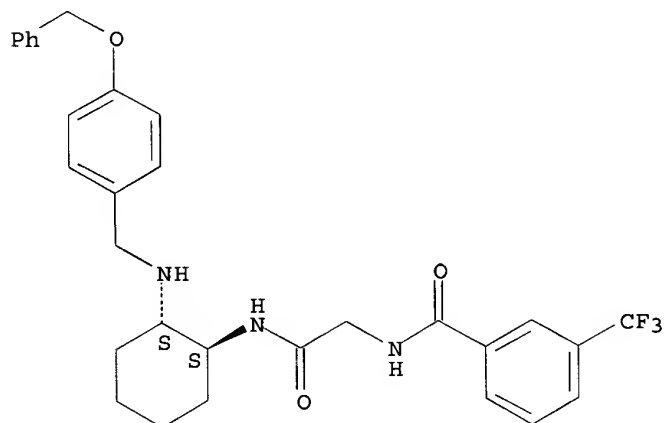




RN 445478-76-2 CAPLUS

CN Benzamide, N-[2-oxo-2-[[[(1S,2S)-2-[[[4-(phenylmethoxy)phenyl]methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

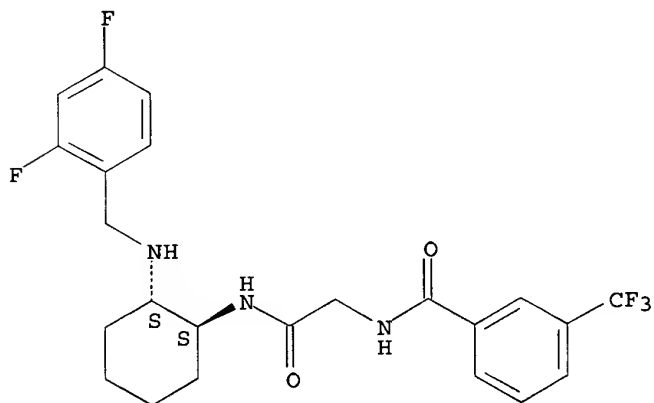
Absolute stereochemistry.

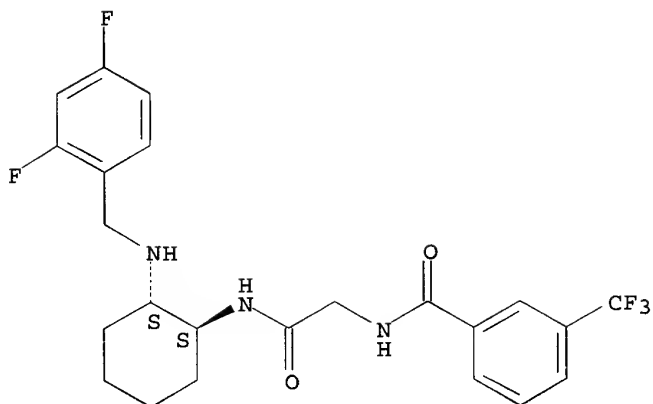


RN 445478-77-3 CAPLUS

CN Benzamide, N-[2-[[[(1S,2S)-2-[[[2,4-difluorophenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

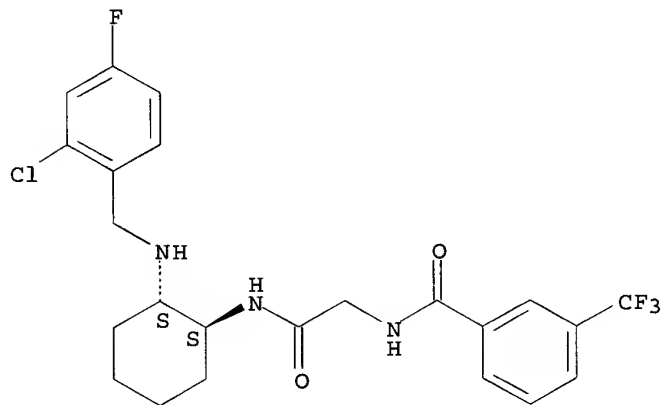




RN 445478-78-4 CAPLUS

CN Benzamide, N-[2-[[[(1S,2S)-2-[[[2-chloro-4-fluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

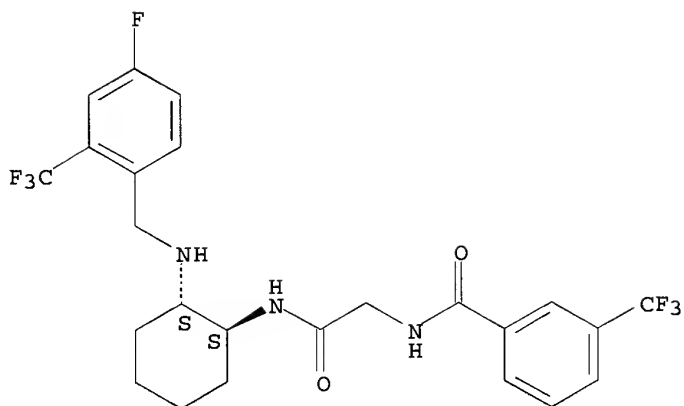
Absolute stereochemistry.



RN 445478-79-5 CAPLUS

CN Benzamide, N-[2-[[[(1S,2S)-2-[[[4-fluoro-2-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

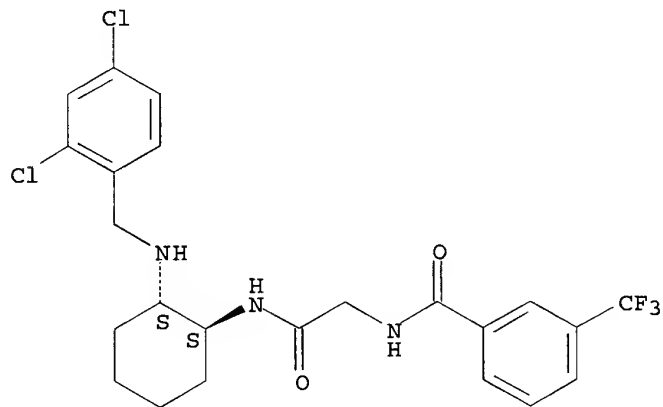
Absolute stereochemistry.



RN 445478-80-8 CAPLUS

CN Benzamide, N-[2-[[[(1S,2S)-2-[[[2,4-dichlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

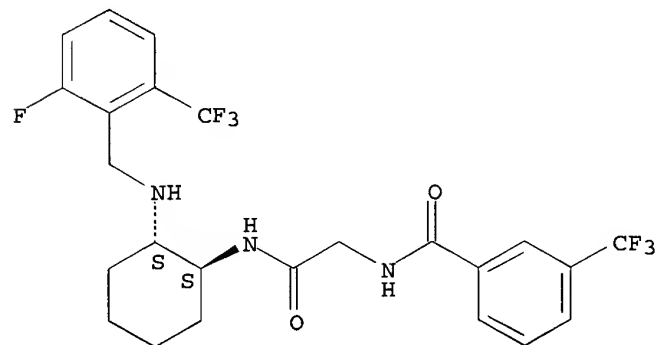
Absolute stereochemistry.



RN 445478-81-9 CAPLUS

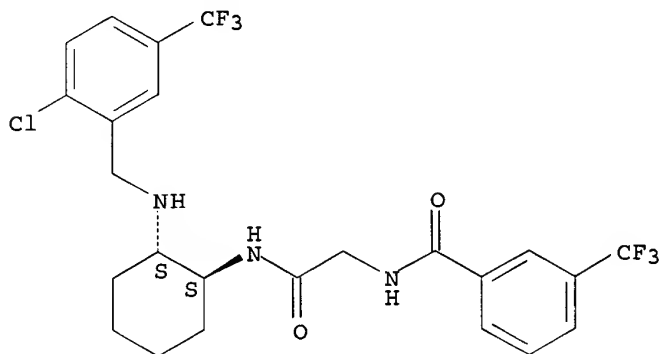
CN Benzamide, N-[2-[[[(1S,2S)-2-[[[2-fluoro-6-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



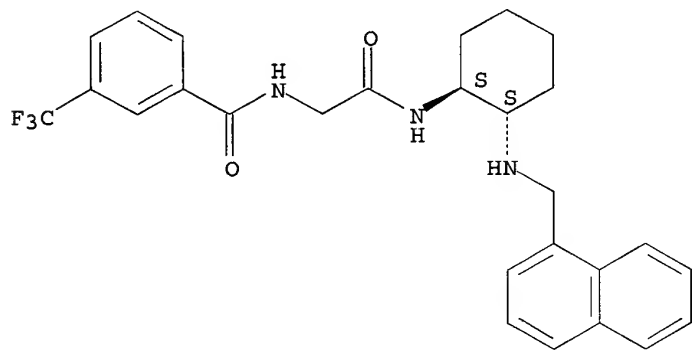
RN 445478-82-0 CAPLUS  
 CN Benzamide, N-[2-[[[(1S,2S)-2-[[[2-chloro-5-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



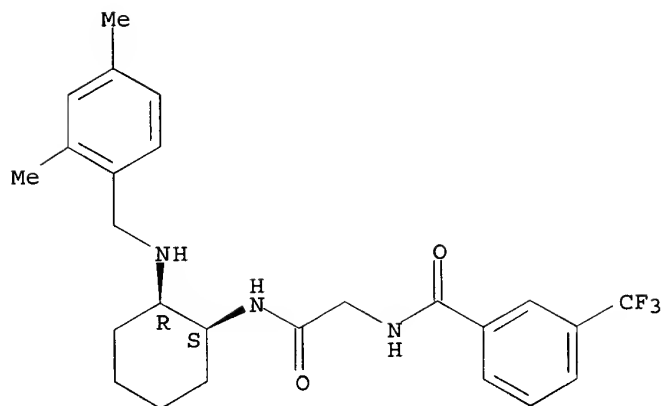
RN 445478-83-1 CAPLUS  
 CN Benzamide, N-[2-[[[(1S,2S)-2-[(1-naphthalenylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 445478-87-5 CAPLUS  
 CN Benzamide, N-[2-[[[(1R,2S)-2-[[[2,4-dimethylphenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

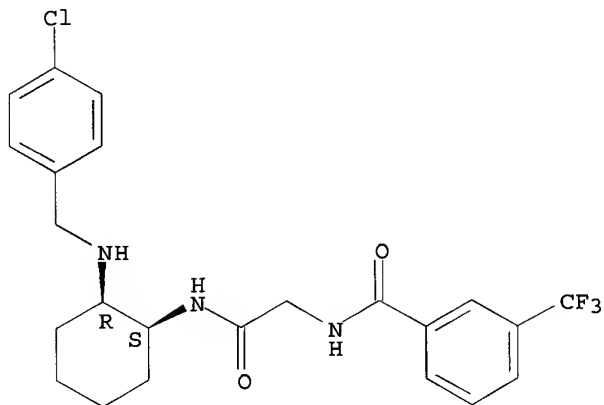
Relative stereochemistry.



RN 445478-88-6 CAPLUS

CN Benzamide, N-[2-[[[(1R,2S)-2-[[[(4-chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

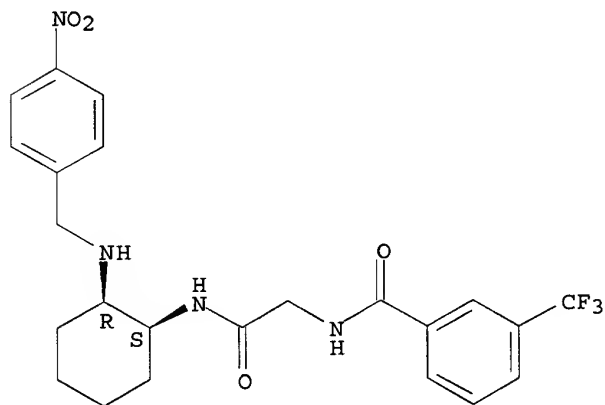
Relative stereochemistry.

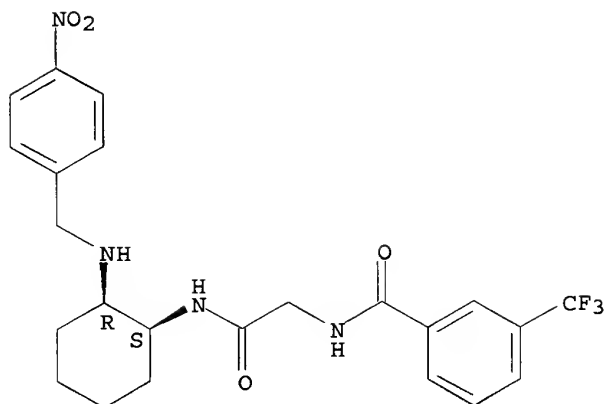


RN 445478-89-7 CAPLUS

CN Benzamide, N-[2-[[[(1R,2S)-2-[[[(4-nitrophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

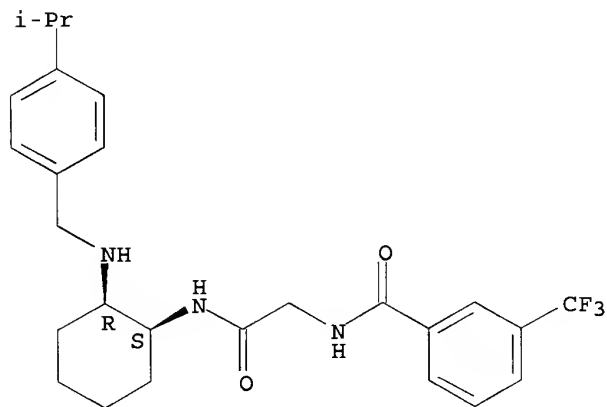




RN 445478-90-0 CAPLUS

CN Benzamide, N-[2-[[[(1R,2S)-2-[[[4-(1-methylethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

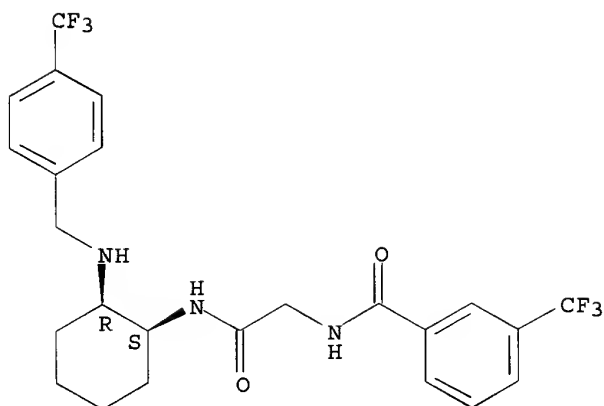
Relative stereochemistry.



RN 445478-91-1 CAPLUS

CN Benzamide, N-[2-oxo-2-[[[(1R,2S)-2-[[[4-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

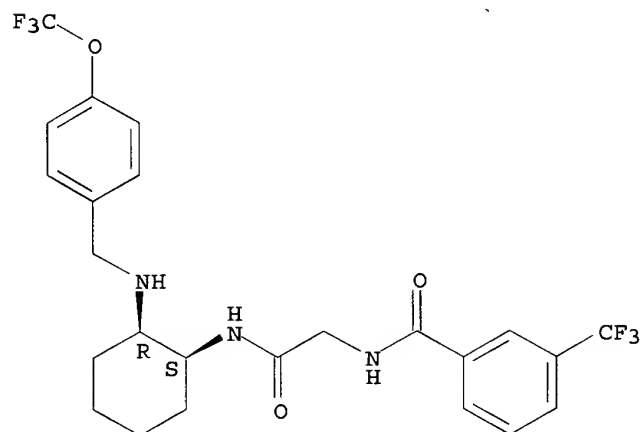
Relative stereochemistry.



RN 445478-92-2 CAPLUS

CN Benzamide, N-[2-oxo-2-[[[(1R,2S)-2-[[[4-(trifluoromethoxy)phenyl]methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

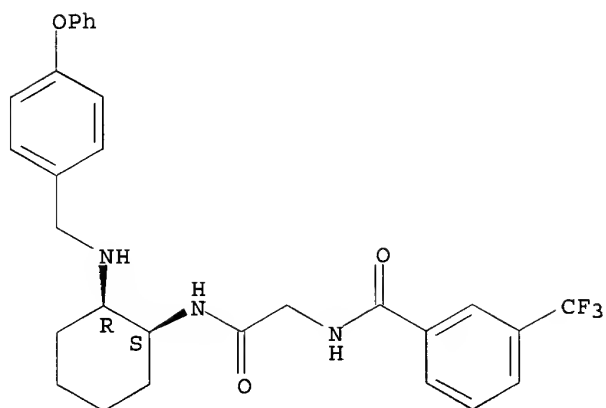
Relative stereochemistry.



RN 445478-93-3 CAPLUS

CN Benzamide, N-[2-oxo-2-[[[(1R,2S)-2-[[[4-phenoxyphenyl]methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

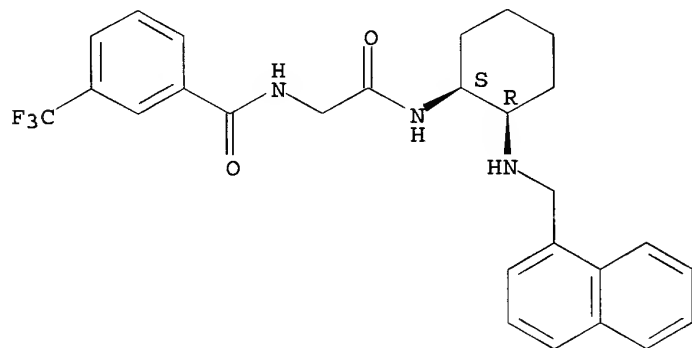
Relative stereochemistry.



RN 445478-94-4 CAPLUS

CN Benzamide, N-[2-[[[(1R,2S)-2-[(1-naphthalenylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

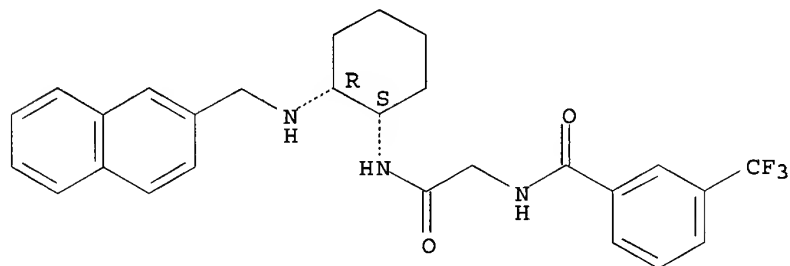
Relative stereochemistry.



RN 445478-95-5 CAPLUS

CN Benzamide, N-[2-[[[(1R,2S)-2-[(2-naphthalenylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

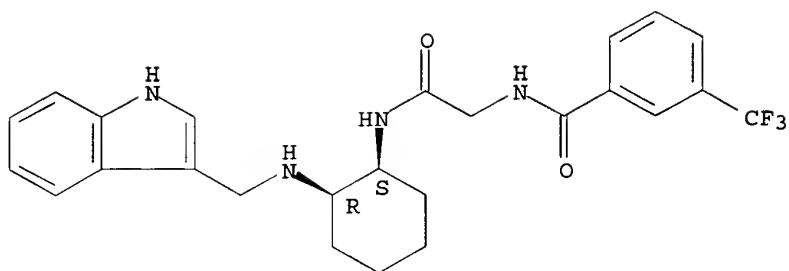


RN 445478-96-6 CAPLUS

CN Benzamide, N-[2-[[[(1R,2S)-2-[(1H-indol-3-ylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

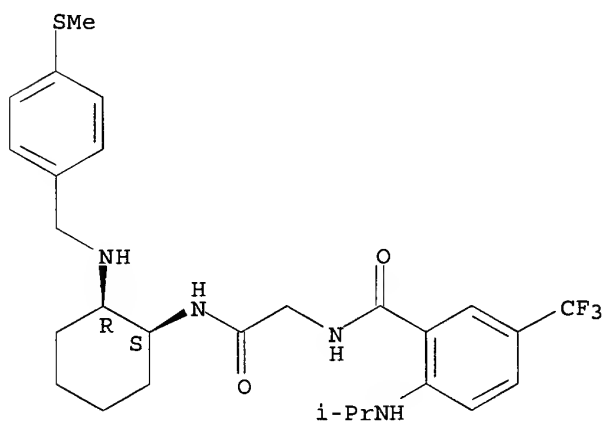




RN 445480-70-6 CAPLUS

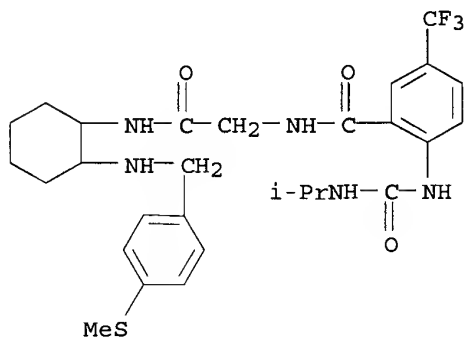
CN Benzamide, 2-[[[(1-methylethyl)amino]carbonyl]amino]-N-[2-[[[(1R,2S)-2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)phenyl]benzamide (9CI) (CA INDEX NAME)

Relative stereochemistry.



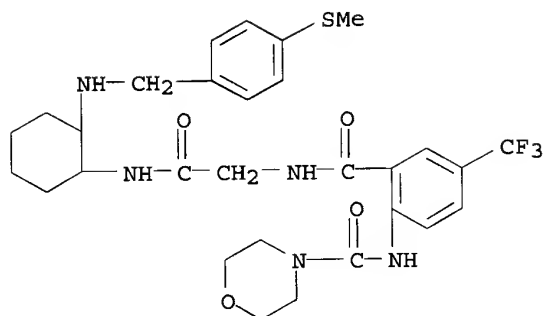
RN 445480-72-8 CAPLUS

CN Benzamide, 2-[[[(1-methylethyl)amino]carbonyl]amino]-N-[2-[[[2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)phenyl]benzamide (9CI) (CA INDEX NAME)



RN 445480-74-0 CAPLUS

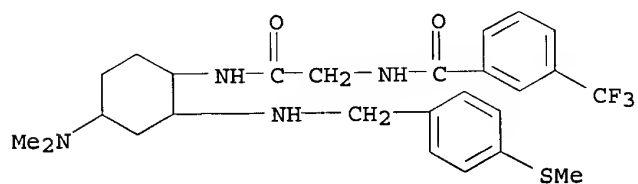
CN 4-Morpholinecarboxamide, N-[2-[[[2-[[[2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]benzamide (9CI) (CA INDEX NAME)



RN 445481-10-7 CAPLUS  
 CN Benzamide, N-[2-[[4-(dimethylamino)-2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

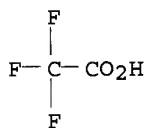
CM 1

CRN 445481-09-4  
 CMF C26 H33 F3 N4 O2 S



CM 2

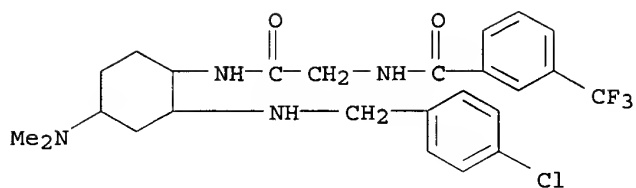
CRN 76-05-1  
 CMF C2 H F3 O2



RN 445481-16-3 CAPLUS  
 CN Benzamide, N-[2-[[2-[[[4-(chlorophenyl)methyl]amino]-4-(dimethylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

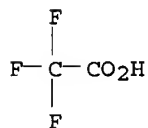
CRN 445481-15-2  
 CMF C25 H30 Cl F3 N4 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



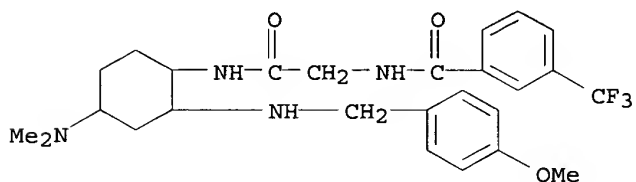
RN 445481-18-5 CAPLUS

CN Benzamide, N-[2-[[4-(dimethylamino)-2-[[[4-methoxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI)  
(CA INDEX NAME)

CM 1

CRN 445481-17-4

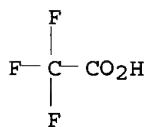
CMF C26 H33 F3 N4 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2

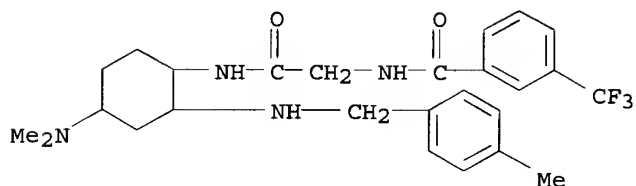


RN 445481-20-9 CAPLUS

CN Benzamide, N-[2-[[4-(dimethylamino)-2-[[[4-methylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

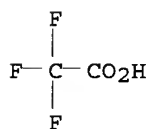
CM 1

CRN 445481-19-6  
CMF C26 H33 F3 N4 O2

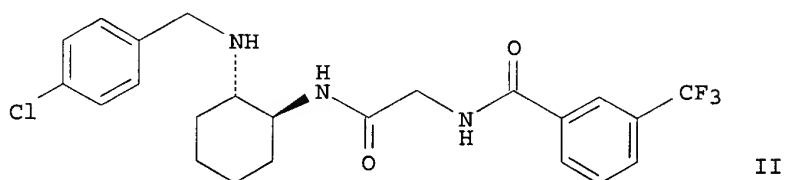
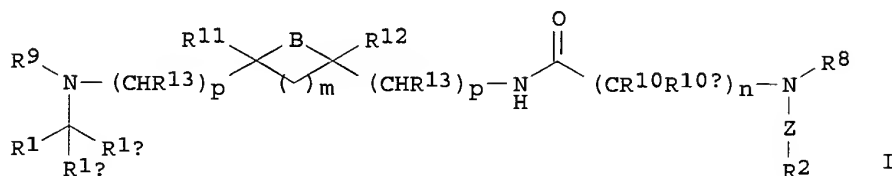


CM 2

CRN 76-05-1  
CMF C2 H F3 O2



GI



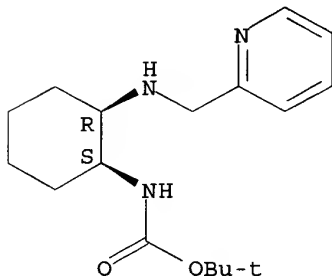
AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepd. as modulators of chemokine receptor activity, esp. monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addn. of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple sclerosis, atherosclerosis and asthma (no data).

L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:220576 CAPLUS  
 DOCUMENT NUMBER: 136:263160  
 TITLE: Preparation of azolylmethylaminotetrahydroquinolines and related compounds as chemokine receptor binding agents.  
 INVENTOR(S): Bridger, Gary; Skerlj, Renato; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Sigiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher  
 PATENT ASSIGNEE(S): Anormed Inc., Can.  
 SOURCE: PCT Int. Appl., 254 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

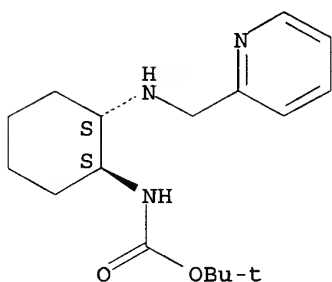
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022600	A2	20020321	WO 2001-CA1326	20010917
WO 2002022600	A3	20020510		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001091569	A5	20020326	AU 2001-91569	20010917
US 2003018046	A1	20030123	US 2001-957682	20010917
PRIORITY APPLN. INFO.:			US 2000-232891P	P 20000915
			US 2000-234510P	P 20000922
			WO 2001-CA1326	W 20010917
OTHER SOURCE(S): MARPAT 136:263160				
IT 405059-09-8P 405175-27-1P 405175-37-3P				
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of azolylmethylaminotetrahydroquinolines and related compds. as chemokine receptor binding agents)				
RN 405059-09-8 CAPLUS				
CN Carbamic acid, [(1R,2S)-2-[(2-pyridinylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)				

Relative stereochemistry.



RN 405175-27-1 CAPLUS  
 CN Carbamic acid, [(1R,2R)-2-[(2-pyridinylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

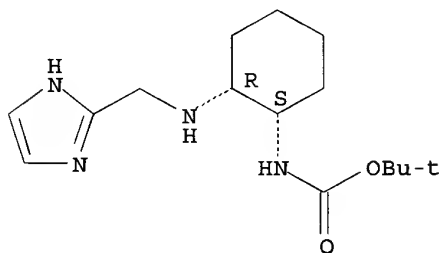
Relative stereochemistry.



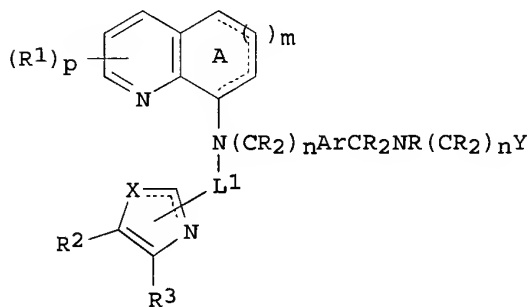
RN 405175-37-3 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[(1H-imidazol-2-ylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



GI



I

AB Title compds. [I; ring A optionally contains N, O, S; dotted lines = optional unsatn.; R1, R2, R3 = non-interfering substituents; p = 0-4; m = 0-2; L1 = linker of 1.5-10 .ANG.; X = O, S, (substituted) C, N; Ar = aryl; n = 0-2; R = H, alkyl; Y = aryl, heteroaryl, heterocyclyl], were prepd. Thus, 5-trifluoromethyl-2-chloromethylbenzimidazole (prepn. given), N-(tert-butoxycarbonyl)-N-(2-pyridinylmethyl)-N'-(5,6,7,8-tetrahydro-8-quinolinyl)-1,4-benzenedimethanamine, and diisopropylethylamine were stirred at 80.degree. in DMF for 16 h to yield N-(tert-butoxycarbonyl)-N-(2-pyridinylmethyl)-N'-(5-trifluoromethyl-1H-benzimidazol-2-ylmethyl)-N'-(5,6,7,8-tetrahydro-8-quinolinyl)-1,4-benzenedimethanamine. Deprotection

with HBr in HOAc or dioxane gave N-(2-pyridinylmethyl)-N'-(5-trifluoromethyl-1H-benzimidazol-2-ylmethyl)-N'-(5,6,7,8-tetrahydro-8-quinolinyl)-1,4-benzenedimethanamine hydrobromide. Several I inhibited HIV-1 replication in MT-4 cells with EC50<20 .mu.g/mL.

L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:220575 CAPLUS

DOCUMENT NUMBER: 136:263159

TITLE: Chemokine receptor-binding heterocyclic compounds, particularly (5,6,7,8-tetrahydroquinolin-8-yl)amino- and (1H-benzimidazol-2-yl)methyl-containing aromatic and heteroaromatic amides, useful for treating infection with HIV and FIV

INVENTOR(S): Bridger, Gary; Skerlj, Renato; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis; Di Fluri, Rosaria Maria

PATENT ASSIGNEE(S): Anormed Inc., Can.

SOURCE: PCT Int. Appl., 146 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022599	A2	20020321	WO 2001-CA1325	20010917
WO 2002022599	A3	20020530		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2001093551	A5	20020326	AU 2001-93551	20010917
US 2002147192	A1	20021010	US 2001-957654	20010917
PRIORITY APPLN. INFO.:			US 2000-233087P P	20000915
			US 2000-234816P P	20000922
			WO 2001-CA1325 W	20010917

OTHER SOURCE(S): MARPAT 136:263159

IT 405059-09-8P, cis-N-(tert-Butoxycarbonyl)-N'-(2-pyridinylmethyl)cyclohexane-1,2-diamine

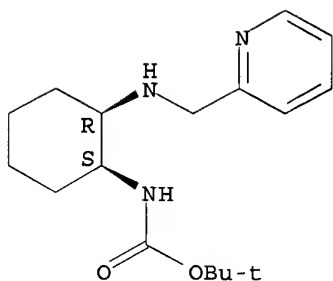
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of tetrahydroquinolinylamino- and benzimidazolylmethyl-contg. heterocyclic amides as chemokine receptor antagonists for treatment of HIV and FIV infection)

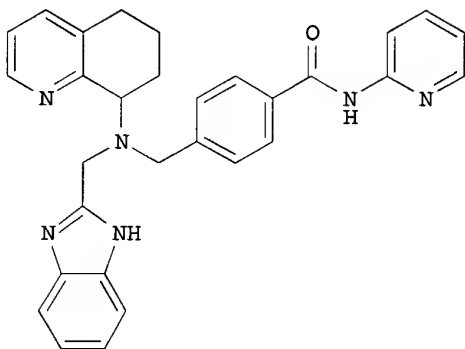
RN 405059-09-8 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[(2-pyridinylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



GI



II

AB Members of a class of (mostly tertiary) amines, contg. a multiplicity of heteroatom. substituents, and the salts and prodrug forms thereof, are useful as chemokine receptor modulators. In particular, compds. of formula X-L1-N(Z)-(CR12)n-Ar-L2-N(R2)-L3-Y (I) are disclosed [wherein: X = monocyclic (5-6 membered) or fused bicyclic (9-12 membered) (un)substituted ring system contg. at least 1 N, O, or S atom; Z = H, monocyclic (5-6 membered) or fused bicyclic (9-12 membered) (un)substituted ring system contg. at least 1 N, O, or S atom; Ar = (un)substituted arom. or heteroatom. ring; each of L1, L2, and L3 = bond, CO, SO2, or CH2, wherein at least 1 of L2 and L3 must comprise CO or SO2, and wherein L1 can also be alkylene (2-5C) wherein 1 or 2 C may optionally be replaced by N and which alkylene may itself optionally be substituted by a bridge alkylene (3-4C); L2 and L3 also may be, independently, SO2NH, CONH, SO2NHCH2 or CONHCH2; n = 0, 1, or 2; each R1 and R2 = H, straight or branched chain or cyclic alkyl (1-6C) which may optionally be substituted, and wherein R2 may be alkylene coupled to Y; and Y comprises at least 1 atom. or heteroatom. or other heterocyclic (un)substituted ring coupled directly to L3]. The compds. are useful for treatment of conditions which are modulated by the chemokine receptors CXCR4 and CCR5, and particularly for treatment of patients infected with HIV or FIV. Examples include 54 syntheses and 3 bioassays, and many addnl. compds. within the invention are listed. For instance, amidation of 4-(chloromethyl)benzoyl chloride with 2-aminopyridine (49%), followed by amination of the chloride with 8-[N-(2-nitrobenzenesulfonyl)amino]-5,6,7,8-tetrahydroquinoline (92%), removal of the 2-nitrobenzenesulfonyl group from the amine using PhSH and K2CO3 in DMF (93%), and finally N-alkylation of the amine with N-BOC-2-(chloromethyl)benzimidazole and deprotection (47%), gave title compd. II, designated AMD 9370. In a test for inhibition of Ca flux induced by the chemokine SDF-1.alpha. in SUP-T1 cells in vitro, 6 compds. including II gave > 20% inhibition at 20 .mu.g/mL. In a test for

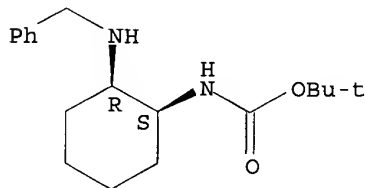


inhibition of NL4.3/IIIB (CXCR4-using) HIV-1 in MT-4 cells in vitro, 7 compds. including II exhibited EC50 values < 20 .mu.g/mL. The compds. also inhibited BaL (CCR5-using) HIV-1 similarly.

L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2001:747751 CAPLUS  
DOCUMENT NUMBER: 135:303902  
TITLE: Preparation of ethylenediamine and  
1,2-cycloalkanediamine derivatives as inhibitors of  
activated blood coagulation factor X  
INVENTOR(S): Yoshino, Toshiharu; Nagata, Tsutomu; Haginoya,  
Noriyasu; Yoshikawa, Kenji; Kanno, Hideyuki;  
Nagamochi, Masatoshi  
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 481 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001074774	A1	20011011	WO 2001-JP2945	20010405
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 2001046835	A5	20011015	AU 2001-46835	20010405
EP 1270557	A1	20030102	EP 2001-919784	20010405
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
NO 2002004766	A	20021128	NO 2002-4766	20021003
PRIORITY APPLN. INFO.:			JP 2000-108047 A	20000405
			WO 2001-JP2945 W	20010405
OTHER SOURCE(S):	MARPAT 135:303902			
IT 365996-39-0P				
RL:	RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)			
	(prepn. of ethylenediamine and cycloalkanediamine derivs. as inhibitors of activated blood coagulation factor X for treatment of thrombosis and embolism)			
RN 365996-39-0	CAPLUS			
CN	Carbamic acid, [(1R,2S)-2-[(phenylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)			

Relative stereochemistry.



AB Compds. of the general formula (1): Q1-Q2-CO-N(R1)-Q3-N(R2)-T1-Q4 [R1, R2 = H, OH, alkyl, alkoxy; Q1 = (un)substituted and (un)satd. 5- to

6-membered cyclohydrocarbonyl or heterocyclyl or bi- or tricyclic condensed heterocyclyl; Q2 = bond, linear or branched alkyl C1-6 alkylene, C2-6 alkenylene, or C2-6 alkynylene, N-alkyl-(un)substituted NH or NH(CH2)m, (un)substituted and (un)satd. divalent 5- to 6-membered cyclic hydrocarbon or heterocycle or bi- or tricyclic condensed heterocycle group; Q3 = CR5R6CR7R8 (wherein R5, R6, R7, R8 = H, HO, halo, haloalkyl, cyano, cyanoalkyl, acyl, acylalkyl, alkyl, alkenyl, alkynyl, alkoxy, alkoxyalkyl, hydroxyalkyl, CO2H, carboxyalkyl, etc.), Q (wherein Q5 = C1-8 alkylene or C2-8 alkenylene; R9 and R10 are substituted on the carbon atoms of the ring contg. Q5 and represent H, OH, alkyl, alkenyl, alkynyl, halo, haloalkyl, cyano, cyanoalkyl, NH2, aminoalkyl, N-alkylaminoalkyl, etc.); Q4 = (un)substituted aryl, arylalkenyl, heteroaryl, or heteroarylalkenyl, (un)substituted and (un)satd. bi- or tricyclic condensed hydrocarbonyl or condensed heterocyclyl; T1 = CO, SO2 are prepd. Also claimed are drugs which contain these compds. and are efficacious for thrombosis and embolism. Thus, (.+-.)-cis-N1 (or N2)-[(5-chloroindol-2-yl)carbonyl]-4,4-(1,2-ethylenedioxy)-1,2-cycloalkanediamine was condensed with 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine-2-carboxylic acid using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and 1-hydroxybenzotriazole monohydrate in DMF at room temp. overnight to give (.+-.)-cis-N1 (or N2)-[(5-chloroindol-2-yl)carbonyl]-4,4-(1,2-ethylenedioxy)-N2 (or N1)-[(5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]-1,2-cyclohexanediamine (II). II in vitro showed IC50 of 1.4 nM .mu.g/mL against human FXa.

REFERENCE COUNT: 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:713294 CAPLUS

DOCUMENT NUMBER: 135:257169

TITLE: Preparation of cyclic .beta.-amino acid derivatives as inhibitors of matrix metalloproteases and TNF-.alpha.

INVENTOR(S): Duan, Jingwu; Ott, Gregory; Chen, Linhua; Lu, Zhonghui; Maduskuie, Thomas P., Jr.; Voss, Matthew E.; Xue, Chu-Biao

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: PCT Int. Appl., 298 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001070673	A2	20010927	WO 2001-US8334	20010315
WO 2001070673	A3	20020314		
W: AT, AU, BR, CA, CH, CN, CZ, DE, DK, EE, ES, FI, HU, IN, JP, KR, LT, LU, LV, MX, NZ, PL, PT, RO, SE, SG, SI, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1263755	A2	20021211	EP 2001-924170	20010315
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR				
US 2002016336	A1	20020207	US 2001-811233	20010316
PRIORITY APPLN. INFO.:				
			US 2000-190182P	P 20000317
			US 2000-233373P	P 20000918
			US 2000-255539P	P 20001214
			WO 2001-US8334	W 20010315

OTHER SOURCE(S): MARPAT 135:257169

IT 362491-59-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

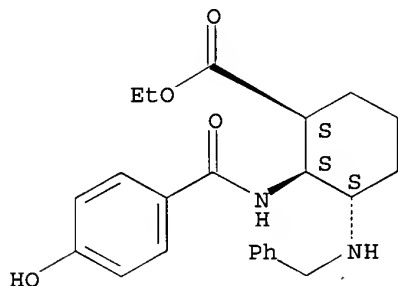
(Reactant or reagent)

(prepn. of cyclic .beta.-amino acid derivs. as inhibitors of matrix metalloproteases and TNF-.alpha.)

RN 362491-59-6 CAPLUS

CN Cyclohexanecarboxylic acid, 2-[(4-hydroxybenzoyl)amino]-3-[(phenylmethyl)amino]-, ethyl ester, (1R,2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AB Novel cyclic .beta.-amino acid derivs. A-CRR2aCRR2bNR1CO-Z-Ua-Xa-Ya-Za [A = CO2H, CH2CO2H, SH, CH2SH, S(O)Ra:NH (Ra = H, alkyl, Ph, benzyl), P(O)(OH)2, etc.; CRR is a substituted 3-13 membered nonarom. carbocyclic or heterocyclic ring; Z is absent or substituted C3-13 carbocycle or 5-14 membered heterocycle; Ua is absent or O, NRa1 (Ra1 = H, alkyl), CO, CO2, O2C, CONRa1, S(O)p (p = 0-2), etc.; Xa is absent or C1-10 alkylene, C2-10 alkenylene or alkynylene; Ya is absent or O, NRa1, S(O)p or CO; Za is H, substituted C3-13 carbocycle or 5-14 membered heterocycle; R1 is H, C1-4 alkyl, Ph, benzyl; R2a is H, C1-6 alkyl, ORa, NRaRa1 or S(O)pRa; R2b is H, C1-6 alkyl (with provisos)] or pharmaceutically acceptable salts were prepd. as metalloprotease and TNF-.alpha. inhibitors. Thus, (3S,4S)-N-hydroxy-1-isopropyl-4-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-3-pyrrolidinecarboxamide was prepd. by a multistep procedure starting with condensation of benzyl Me maleate, glycine, and paraformaldehyde to form 3,4-pyrroledicarboxylate diester and involving amidation of 4-[(2-methyl-4-quinolinyl)methoxy]benzoic acid.

L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:836249 CAPLUS

DOCUMENT NUMBER: 134:147352

TITLE: Amide catalysts with tetradentate ligands and the asymmetric transfer hydrogenation of carbonyl compounds

AUTHOR(S): Marson, C. M.; Schwarz, I.

CORPORATE SOURCE: Department of Chemistry, University College London, Christopher Ingold Laboratories, London, WC1H 0AJ, UK

SOURCE: Tetrahedron Letters (2000), 41(46), 8999-9003

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:147352

IT 323187-53-7P 323187-54-8P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);

USES (Uses)

(prepn. of amidic tetradentate ligands as catalysts for asym. transfer hydrogenation of carbonyl compds.)

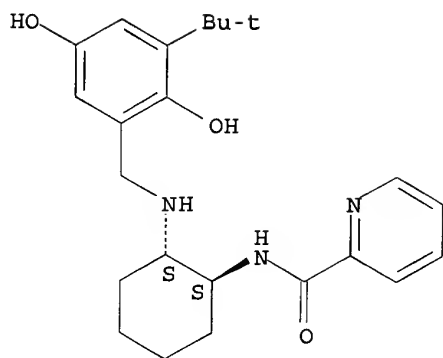
RN 323187-53-7 CAPLUS

CN Ethanediame, N,N'-bis[(1R,2R)-2-[(phenylmethyl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Chemical structure of a bis-amine compound, likely a ligand for a metal complex. The structure features a central amide linkage ( $\text{C}(=\text{O})\text{NH}\text{C}(=\text{O})\text{NH}$ ) connecting two cyclohexane rings. Each cyclohexane ring is substituted with two 'R' groups and one 'NH-Ph' group. The stereochemistry is indicated with wedges and dashes.

L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 1999:251901 CAPLUS  
DOCUMENT NUMBER: 131:10019  
TITLE: Discovery of novel catalysts for alkene epoxidation  
from metal-binding combinatorial libraries  
AUTHOR(S): Francis, Matthew B.; Jacobsen, Eric N.  
CORPORATE SOURCE: Department of Chemistry and Chemical Biology and  
Institute of Chemistry and Cellular Biology, Harvard  
University, Cambridge, MA, 02138, USA  
SOURCE: Angewandte Chemie, International Edition (1999),  
38(7), 937-941  
CODEN: ACIEF5; ISSN: 1433-7851  
PUBLISHER: Wiley-VCH Verlag GmbH  
DOCUMENT TYPE: Journal  
LANGUAGE: English

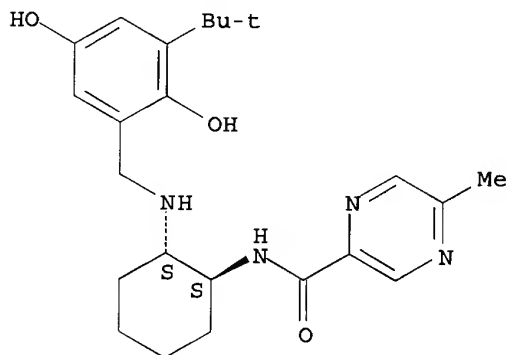
Absolute stereochemistry.



RN 225666-17-1 CAPLUS

CN Pyrazinecarboxamide, N-[(1S,2S)-2-[[[3-(1,1-dimethylethyl)-2,5-dihydroxyphenyl]methyl]amino]cyclohexyl]-5-methyl- (9CI) (CA INDEX NAME)

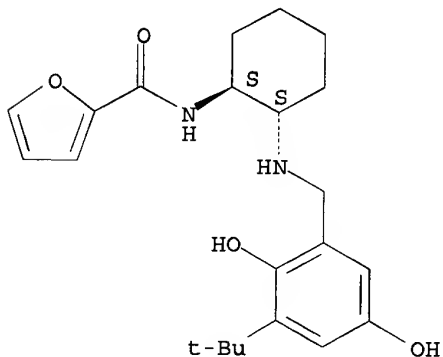
Absolute stereochemistry.



RN 225666-18-2 CAPLUS

CN 2-Furancarboxamide, N-[(1S,2S)-2-[[[3-(1,1-dimethylethyl)-2,5-dihydroxyphenyl]methyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

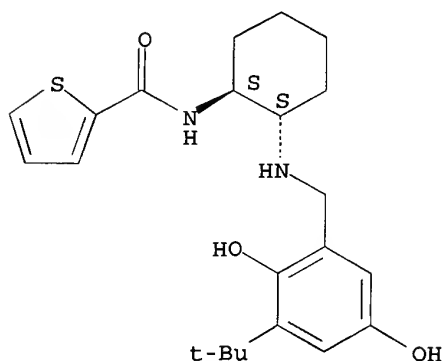
Absolute stereochemistry.



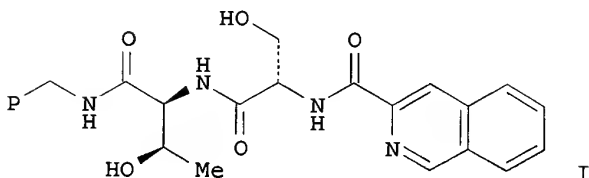
RN 225666-19-3 CAPLUS

CN 2-Thiophenecarboxamide, N-[(1S,2S)-2-[[[3-(1,1-dimethylethyl)-2,5-dihydroxyphenyl]methyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



AB A combinatorial library of imine ligands is prepd. on solid support and tested for activity in the stereoselective epoxidn. of trans-.beta.-methylstyrene in the presence of metal salts and hydrogen peroxide. The library consisted in part of amino acids (asparagine, cysteine, histidine, methionine, or serine) linked at their N-termini to cis-aminoindenol, trans-diaminocyclohexane, or serine whose free amino groups were used to form imines or amides with aldehydes or carboxylic acids. A library of salen ligands with different imine groups was also prepd. FeCl<sub>2</sub> was the most effective metal precursor with the libraries in epoxidns. with H<sub>2</sub>O<sub>2</sub>. Serine or cysteine worked best as the C-terminal amino acids for epoxidn. ligands, while 2-pyridinecarboxaldehyde and 2-pyridinecarboxylic acid were the most effective capping reagents for the ligands. Polymer-bound ligand I (P = polymer) was treated with a 0.02M soln. of FeCl<sub>2</sub> in 4:1 THF:MeOH and agitated and purified until the THF:MeOH rinses were clear; treatment of trans-.beta.-methylstyrene in 1:1 CH<sub>2</sub>Cl<sub>2</sub>:Me<sub>3</sub>COH with the resin-bound FeCl<sub>2</sub> complex of I followed by addn. of 1.5 equiv. of 30% H<sub>2</sub>O<sub>2</sub> gave (R,R)-trans-.beta.-methylstyrene oxide with 78% conversion, 69% yield, and in 20% ee.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1981:103032 CAPLUS

DOCUMENT NUMBER: 94:103032

TITLE: Analgesic N-(2-(furylmethylamino and 2-thienylmethylamino)cycloaliphatic)benzamides

INVENTOR(S): Szmuszkovic, Jacob

PATENT ASSIGNEE(S): Upjohn Co., USA

SOURCE: U.S., 33 pp. Cont.-in-part of U.S. 4,153,717.  
CODEN: USXXAM

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

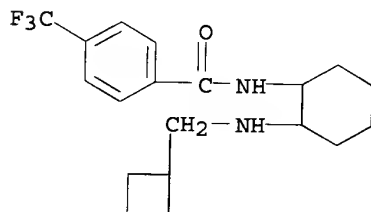
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4215114	A	19800729	US 1979-17679	19790305
US 4098904	A	19780704	US 1976-741467	19761112
CA 1072558	A1	19800226	CA 1977-287430	19770926
US 4153717	A	19790508	US 1978-906271	19780515
US 4192885	A	19800311	US 1979-18550	19790308
PRIORITY APPLN. INFO.:			US 1976-741467	19761112
			US 1978-906271	19780515
			US 1978-904477	19780510
			CA 1979-287430	19790906

IT 75570-55-7P

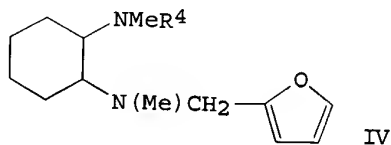
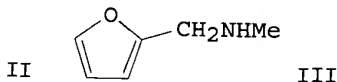
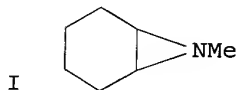
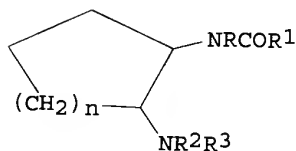
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 75570-55-7 CAPLUS

CN Benzamide, N-[2-[(cyclobutylmethyl)amino]cyclohexyl]-4-(trifluoromethyl)-  
 (9CI) (CA INDEX NAME)



GI



AB Analgesic (no data) cycloaliph. benzamides I ( $n = 1-8$ ;  $R = H$ , alkyl;  $R_1 =$  optionally substituted Ph;  $R_2 =$  alkyl;  $R_3 =$  furfuryl, thenyl) were prepd. Thus, heating II with furfurylamine III gave IV ( $R_4 = H$ ) which was acylated using 3,4-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>COCl to IV ( $R_4 =$  COC<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>-3,4).

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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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ENTRY	SESSION
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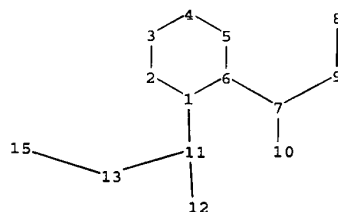
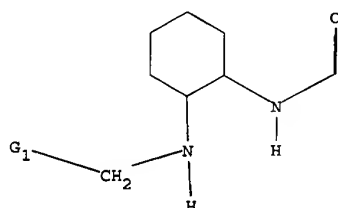
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ing nodes :

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main bonds :

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ing bonds :

1-2 1-6 2-3 3-4 4-5 5-6

act/norm bonds :

1-11 6-7 7-9 8-9 13-15

act bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-10 11-12 11-13

olated ring systems :

containing 1 :

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atch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 15:CLASS